# **CLAIMS**

1. A compound of the formula

$$\begin{array}{c|c}
 & O \\
 & M & N & A_1 \\
 & N & Y & A_2 \\
 & N & Y & A_2
\end{array}$$

$$\begin{array}{c}
 & A_1 \\
 & A_2 \\
 & Y & A_2
\end{array}$$

wherein  $A_1$ , each  $A_2$  (if present), and  $A_3$  are independently selected from  $C_1$ -  $C_8$  alkyl;

wherein each Y is independently selected from H or  $C_1$ - $C_4$  alkyl; wherein M is selected from  $C_1$ - $C_4$  alkyl; wherein k is 0, 2, or 3; and wherein R is selected from  $C_1$ - $C_{32}$  alkyl; and all stereoisomers and salts thereof.

- 2. A compound according to claim 1, wherein each Y group is -H.
- 3. A compound according to claim 1, wherein each Y group is -CH<sub>3</sub>.
- 4. A compound according to claim 1, wherein  $A_1$ , each  $A_2$  (if present), and  $A_3$  are independently selected from  $C_2$ - $C_4$  alkyl.
  - 5. A compound according to claim 1, wherein M is -CH<sub>2</sub>-.

### 6. A compound of the formula

$$\begin{array}{c|c}
 & O \\
 & M \\
 & N \\
 & Y \\
 & N \\
 & N \\
 & Y \\
 & N \\
 & Y \\
 & N \\$$

wherein  $A_1$  and  $A_3$  are independently selected from  $C_1$ - $C_8$  alkyl; wherein  $A_2$  is independently selected from  $C_1$ - $C_3$  alkyl or  $C_5$ - $C_8$  alkyl; wherein each Y is independently selected from H or  $C_1$ - $C_4$  alkyl; wherein M is selected from  $C_1$ - $C_4$  alkyl; and wherein R is selected from  $C_1$ - $C_{32}$  alkyl; and all stereoisomers and salts thereof.

- 7. A compound according to claim 6, wherein each Y group is -H.
- 8. A compound according to claim 6, wherein each Y group is -CH<sub>3</sub>.
- 9. A compound according to claim 6, wherein  $A_1$  and  $A_3$  are independently selected from  $C_2$ - $C_4$  alkyl, and  $A_2$  is selected from the group consisting of  $C_2$ - $C_3$  alkyl and  $C_5$  alkyl.
  - 10. A compound according to claim 6, wherein M is -CH<sub>2</sub>-.

# 11. A compound of the formula

$$\begin{array}{c|c}
 & O \\
 & & A_1 \\
 & & N \\
 & & Y \\
 & & A_3 \\
 & & & N \\
 & & & & A_2
\end{array}$$

wherein  $A_1$  and  $A_3$  are independently selected from  $C_1$ - $C_8$  alkyl; wherein  $A_2$  is independently selected from  $C_1$ - $C_8$  alkyl; wherein each Y is independently selected from H or  $C_2$ - $C_4$  alkyl; wherein M is selected from  $C_1$ - $C_4$  alkyl; and wherein R is selected from  $C_1$ - $C_{32}$  alkyl; and all stereoisomers and salts thereof.

- 12. A compound according to claim 11, wherein each Y group is -H.
- 13. A compound according to claim 11, wherein  $A_1$  and  $A_3$  are independently selected from  $C_2$ - $C_4$  alkyl, and  $A_2$  is selected from the group consisting of  $C_2$ - $C_5$  alkyl.
  - 14. A compound according to claim 11, wherein M is -CH<sub>2</sub>-.

# 15. A method of synthesizing a compound of the formula

$$\begin{bmatrix} & & & & & \\ & & & & & \\ & & & & & \\ & & & & & \\ & & & & & \\ & & & & & \\ & & & & & \\ & & & & & \\ & & & & & \\ & & & & & \\ & & & & & \\ & & & & & \\ & & & & & \\ & & & & & \\ & & & & & \\ & & & & & \\ & & & & & \\ & & & & & \\ & & & & & \\ & & & & & \\ & & & & & \\ & & & & & \\ & & & & & \\ & & & & & \\ & & & & & \\ & & & & & \\ & & & & & \\ & & & & & \\ & & & & & \\ & & & & & \\ & & & & & \\ & & & & & \\ & & & & & \\ & & & & & \\ & & & & & \\ & & & & & \\ & & & & & \\ & & & & & \\ & & & & & \\ & & & & & \\ & & & & & \\ & & & & & \\ & & & & & \\ & & & & & \\ & & & & & \\ & & & & & \\ & & & & & \\ & & & & & \\ & & & & & \\ & & & & & \\ & & & & & \\ & & & & & \\ & & & & & \\ & & & & & \\ & & & & & \\ & & & & & \\ & & & & & \\ & & & & & \\ & & & & \\ & & & & \\ & & & & \\ & & & & \\ & & & & \\ & & & & \\ & & & & \\ & & & & \\ & & & & \\ & & & & \\ & & & & \\ & & & & \\ & & & & \\ & & & & \\ & & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & &$$

wherein  $A_1$ , each  $A_2$  (if present), and  $A_3$  are independently selected from  $C_1$ - $C_8$  alkyl;

wherein each Y is independently selected from H or C<sub>1</sub>-C<sub>4</sub> alkyl;

wherein M is selected from C<sub>1</sub>-C<sub>4</sub> alkyl;

wherein k is 0, 1, 2, or 3;

and wherein R is selected from C<sub>1</sub>-C<sub>32</sub> alkyl;

comprising the steps of:

reacting an  $\omega$ -halo alkyl alkanoate with an aldehyde or ketone-containing compound to give an alkene-containing alkanoate compound;

reacting the alkene-containing alkanoate compound with a compound containing two primary amino groups and optionally containing secondary amino groups to effect addition of one of the amino groups across the double bond;

cyclizing the other amino group with the alkanoate group to form an amide bond; and

optionally alkylating the secondary amino groups if present.

- 16. The method of claim 15, wherein the  $\omega$ -halo alkyl alkanoate is ethyl bromoacetate.
- 17. The method of claim 16, wherein the aldehyde or ketone-containing compound is an aldehyde-containing compound.

- 18. The method of claim 16, wherein the step of reacting an  $\omega$ -halo alkyl alkanoate with an aldehyde or ketone-containing compound to give an alkene-containing alkanoate compound is performed by reacting the  $\omega$ -halo alkyl alkanoate with triphenylphosphine.
- 19. The method of claim 16, wherein the compound containing two primary amino groups is selected from the group consisting of H<sub>2</sub>N-A<sub>1</sub>-(NH-A<sub>2</sub>)<sub>k</sub>-NH-A<sub>3</sub>-NH<sub>2</sub> wherein A<sub>1</sub>, each A<sub>2</sub> (if present), and A<sub>3</sub> are independently selected from C<sub>1</sub>-C<sub>8</sub> alkyl and k is 0, 1, 2, or 3.
- 20. The method of claim 19, wherein the compound containing two primary amino groups is selected from the group consisting of spermine, spermidine, and putrescine.
- 21. The method of claim 16, wherein the step of cyclizing the other amino group with the alkyl alkanoate group to form an amide bond is performed by reacting the compound with antimony (III) ethoxide.
- 22. The method of claim 16, wherein the step of optionally alkylating any secondary amino groups if present is performed by reacting the compound first with an aliphatic aldehyde to result in a Schiff base, then reducing the Schiff base, resulting in alkylation of the secondary amino groups.
- 23. The method of claim 22, wherein the step of reducing the Schiff base is performed by using the reagent NaCNBH<sub>3</sub>.
  - 24. A method of synthesizing a compound of the formula

$$\begin{array}{c|c}
 & O \\
 & N \\
 & N \\
 & Y \\
 & N \\$$

wherein  $A_1$  is  $C_3$  alkyl, and each  $A_2$  (if present) and  $A_3$  are independently selected from  $C_1$ - $C_8$  alkyl;

wherein each Y is independently selected from H or C<sub>1</sub>-C<sub>4</sub> alkyl;

wherein M is selected from C<sub>1</sub>-C<sub>4</sub> alkyl;

wherein k is 0, 1, 2, or 3;

and wherein R is selected from C<sub>1</sub>-C<sub>32</sub> alkyl;

comprising the steps of:

condensing a compound comprising a primary amino group and a hexahydropyrimidine moiety with an  $\alpha$ , $\beta$ -unsaturated ester compound such that the primary amino group adds at the  $\beta$ -position of the unsaturated ester compound, whereby the primary amino group is converted to a secondary amino group;

cleaving the methylene bridge of the hexahydropyrimidine moiety to generate a secondary amino group and a newly-generated primary amino group; and

condensing the newly-generated primary amino group with the ester group to form an amide group.

25. The method of claim 24, wherein the  $\alpha,\beta$ -unsaturated ester is of the formula

 $(C_1-C_8 \text{ alkyl})-O-C(=O)-CH=CH-(C_1-C_{32} \text{ alkyl}).$ 

26. The method of claim 24, wherein the compound comprising a primary amino group and a hexahydropyrimidine moiety is of the formula

$$H_2N-A_3-(NY-A_2)_j-N$$
NH

wherein each  $A_2$  (if present) and  $A_3$  are independently selected from  $C_1\text{-}C_8$  alkyl;

wherein each Y is independently selected from H or  $C_1$ - $C_4$  alkyl; and wherein j is 0, 1, 2, or 3.

- 27. The method of claim 26, wherein j is 0.
- 28. The method of 27, wherein  $A_3$  is  $C_4$  alkyl.
- 29. The method of 24, wherein the step of cleaving the methylene bridge of the hexahydropyrimidine moiety is performed with anhydrous HCl in an alcoholic solvent.
- 30. The method of 24, wherein the step of condensing the newly-generated primary amino group with the ester group to form an amide group is performed with the reagent  $B(N(CH_3)_2)_3$ .
- 31. A method of treating cancer or a disease characterized by uncontrolled cell proliferation in an individual in need of such treatment,

comprising the step of administering one or more compounds of claim 1.

32. A method of treating cancer or a disease characterized by uncontrolled cell proliferation in an individual in need of such treatment,

comprising the step of administering one or more compounds of claim 6.

33. A method of treating cancer or a disease characterized by uncontrolled cell proliferation in an individual in need of such treatment,

comprising the step of administering one or more compounds of claim 11.

- 34. A method of depleting ATP in a cancerous cell, comprising the step of administering one or more compounds of claim 1 to the cell.
- 35. A method of depleting ATP in a cancerous cell, comprising the step of administering one or more compounds of claim 6 to the cell.
- 36. A method of depleting ATP in a cancerous cell, comprising the step of administering one or more compounds of claim 11 to the cell.

#### 37. A compound of the formula

$$\begin{array}{c}
X \\
A_4 \\
A_1 \\
NY \\
A_3 \\
NY \\
A_2
\end{array}$$

$$\begin{array}{c}
X \\
NY \\
A_2
\end{array}$$

$$\begin{array}{c}
X \\
NY \\
A_2
\end{array}$$

wherein  $A_1$ , each  $A_2$  (if present), and  $A_3$  are independently selected from  $C_1$ - $C_8$  alkyl;

wherein A<sub>4</sub> is selected from C<sub>1</sub>-C<sub>8</sub> alkyl or a nonentity;

X is selected from -H, -Z, -CN, -NH<sub>2</sub>, -C(=O)-C<sub>1</sub>-C<sub>8</sub> alkyl, or -NHZ, with the proviso that when A<sub>4</sub> is a nonentity, X is -H, -C(=O)-C<sub>1</sub>-C<sub>8</sub> alkyl, or -Z;

Z is selected from the group consisting of an amino protecting group, an amino capping group, an amino acid, and a peptide;

wherein each Y is independently selected from H or  $C_1$ - $C_4$  alkyl; wherein M is selected from  $C_1$ - $C_4$  alkyl; wherein k is 0, 1, 2, or 3; and wherein R is selected from  $C_1$ - $C_{32}$  alkyl; and all stereoisomers and salts thereof.

- 38. The compound of claim 37, wherein  $A_4$  is a nonentity, X is -Z, -Z is -H, and each Y is - $CH_3$ .
- 39. The compound of claim 38, wherein M is -CH<sub>2</sub>-, k is 1, A<sub>1</sub> and A<sub>3</sub> are -CH<sub>2</sub>CH<sub>2</sub>CH<sub>2</sub>-, and the single A<sub>2</sub> group is -CH<sub>2</sub>CH<sub>2</sub>CH<sub>2</sub>CH<sub>2</sub>-.
  - 40. The compound of claim 39, wherein R is  $-C_{13}H_{27}$ .
- 41. The compound of claim 37, wherein  $A_4$  is  $C_1$ - $C_8$  alkyl, X is -NHZ, and and Z is selected from one of the 20 genetically encoded amino acids, a peptide of the formula acetyl-SKLQL-, a peptide of the formula acetyl-SKLQ- $\beta$ -alanine-, or a peptide of the formula acetyl-SKLQ-.
- 42. A method of synthesizing a compound of claim 37, wherein  $A_4$  is a nonentity and X is -H, comprising reducing the carbonyl of the amide group of a compound of the formula

$$\begin{array}{c|c}
X \\
O & A_4 \\
A_1 \\
N & A_1 \\
N & A_2 \\
N & Y
\end{array}$$

$$\begin{array}{c}
A_1 \\
A_2 \\
A_2
\end{array}$$

$$\begin{array}{c}
A_3 \\
N \\
Y
\end{array}$$

wherein A<sub>4</sub> is a nonentity and X is -H.

43. A method of synthesizing a compound of claim 37, wherein  $A_4$  is  $C_2$  alkyl, each Y is selected from  $C_1$ - $C_4$  alkyl, and X is -CN, comprising reacting a compound of the formula

$$\begin{array}{c|c}
M & & H \\
N & & A_1 \\
N & & A_2 \\
N & & & Y
\end{array}$$

wherein each Y is selected from  $C_1$ - $C_4$  alkyl, with a compound of the formula  $H_2C$ =CH-CN.

44. A method of synthesizing a compound of claim 37, wherein  $A_4$  is  $C_3$  alkyl and X is -NH<sub>2</sub>, comprising reducing the nitrile group of a compound of the formula

$$\begin{array}{c|c}
CN \\
A_4 \\
A_1 \\
NY \\
A_3 \\
NY \\
A_2
\end{array}$$

where  $A_4$  is selected from  $C_1$ - $C_7$  alkyl, to an amino group.